Summer Program FGV/EMAp 2019

Introduction to Machine Learning with Python

Regression Models

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Basic Concepts

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Properly estimating the parameters β_j is the main goal of a linear regression.

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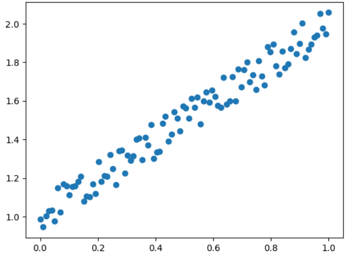

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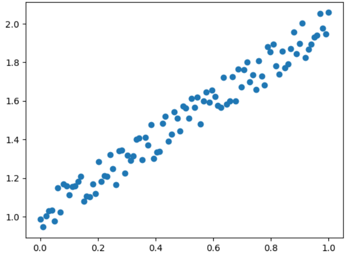
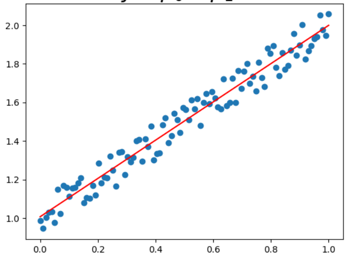


$$y = \beta_0 + \beta_1 x$$



Residual Sum of Squares

The **least squares** method computes the parameters $\boldsymbol{\beta} = (\beta_0, \beta_1, \ldots, \beta_d)^\top$ so as to minimize the **residual sum of squares**

$$RSS(\boldsymbol{\beta}) = \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i))^2 = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{d} x_{ij}\beta_j \right)^2$$

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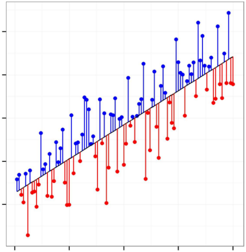

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$$RSS(\boldsymbol{\beta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Residual Sum of Squares

Differentiating $RSS(\boldsymbol{\beta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$ with respect to $\boldsymbol{\beta}$ and setting the derivative to zero

$$\frac{\partial RSS(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = 0 \Rightarrow \mathbf{X}^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = 0$$

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$$\boxed{\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}}$$

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In practice $\hat{\boldsymbol{\beta}}$ is computed solving the system $(\mathbf{X}^\top\mathbf{X})\boldsymbol{\beta} = \mathbf{X}^\top\mathbf{y}$ (using QR factorization).

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Considering the *mean square error* and assuming $\hat{\boldsymbol{\beta}}$ an estimate (not necessarily the least squares) we have

$$MSE(\hat{\boldsymbol{\beta}}) = E(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^2 = \underbrace{Var(\hat{\boldsymbol{\beta}})}_{variance} + \underbrace{\left[E(\hat{\boldsymbol{\beta}}) - \boldsymbol{\beta}\right]^2}_{\substack{bias \\ (=0 \text{ for unbiased})}}$$

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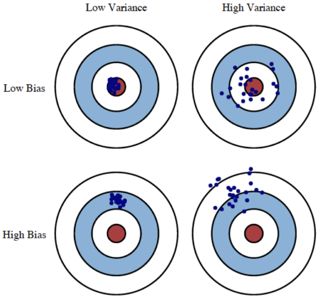

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There are several ways to obtain such biased estimates !!

– *subset selection*

– *regularized optimization schemes*

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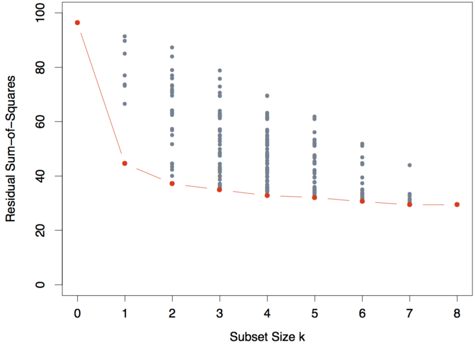

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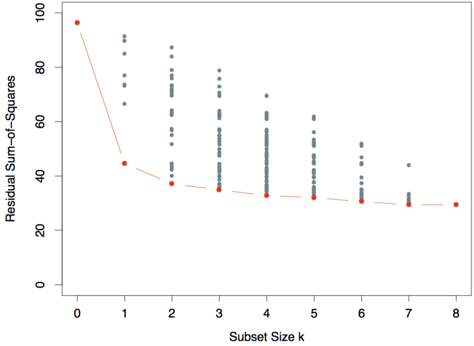

Computationally unfeasible for large values of d !!

Forward- and Backward-Stepwise

Greedy-like alternatives to reduce the computational burden !!

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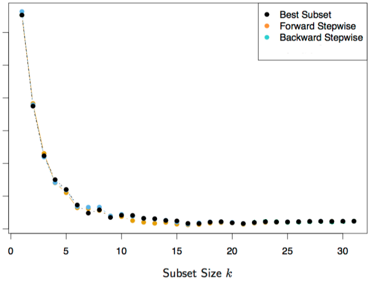

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The idea is play with the full model, but imposing penalties to the parameters so as to shrink them to zero.

Ridge Regression

$$\hat{\boldsymbol{\beta}} = \operatorname{argmin}_{\beta} \left\{ \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{d} x_{ij}\beta_j)^2 + \ s \sum_{j=1}^{d} \beta_j^2 \ \right\}$$

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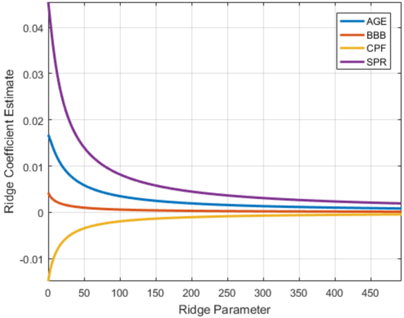

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Without β_0 we can write the residual sum of squares as:

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Differentiating w.r.t. $\boldsymbol{\beta}$ and setting the derivative to zero we get

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X} + s\mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$$

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$$\mathbf{y} \sim \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}^\top\mathbf{X} + s\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{y} \tag{1}$$

$$= \sum_{j=1}^{p} \mathbf{u}_j \, \frac{d_j^2}{d_j^2 + s} \, \mathbf{u}_j^\top \mathbf{y} \tag{2}$$

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The smaller d_j and larger s the closer to zero $\frac{d_j^2}{d_j^2+s}$ is.
Since small d_j are related to noise (remember PCA lesson !), rigde regression is making a "soft" selection of the main components, removing noise and writing data back in the original coordinate system.

Lasso

Lasso is similar to ridge regression,

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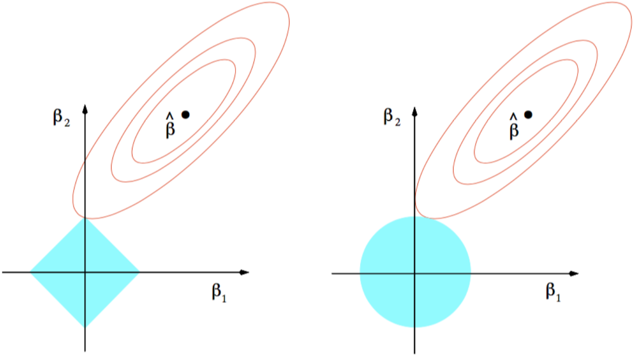
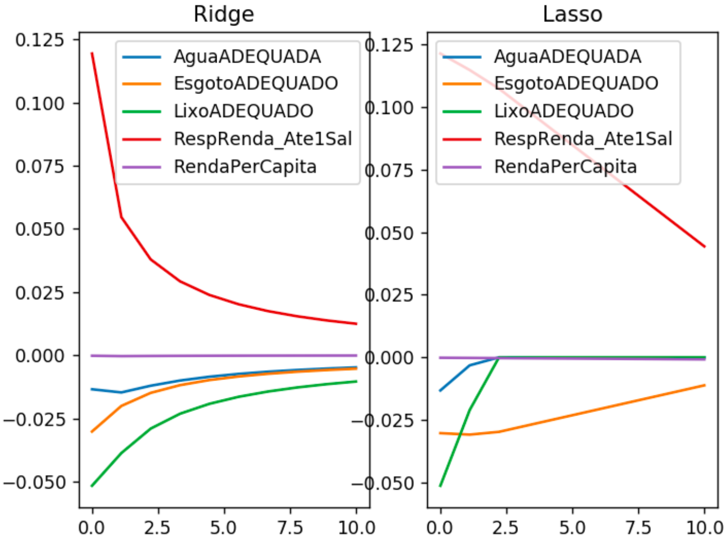
Unfortunately there is no closed form expression for the solution of the Lasso regression, thus a optimization procedure has to be employed to compute $\hat{\boldsymbol{\beta}}$.

Lasso

An import aspect of Lasso is that, tuning s properly, non-relevant parameters are quickly truncated to zero.



Lasso x Rigde



Cross-Validation

K-fold approach:

D1	D2	D3	D4	D5
Train	Train	Validation	Train	Train

Given a model M and a K-fold of a data set D

- for $k = 1, \ldots, K$
  - Consider the training set $D^{(-k)} = D/D_k$
  - Learn M from $D^{(-k)}$
  - $e_k(M) = \sum_{i \in D_k} (y_i - \hat{y}_i^{(-k)})^2$
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When $K = n$ the K-fold is called *leave-one-out cross-validation*.

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K-fold can be used to assess the quality of a particular model.